Compatibility of Distortion Fields Caused by Topological Defects in 2D Lattices

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Abstract. – Topological defects in crystalline lattices are considered. In relation to physical realizability of such defects, criteria for geometric compatibility of the lattice distortions are formulated. For 2D lattices it is shown that the answer to the question of existence of distortion fields which are both geometrically compatible and homotopically non–trivial is in the affirmative.

1 Introduction

Since the paper [1] which first introduced homotopy into physics, considerable interest in topologically non–trivial configurations of physical systems has arisen. In particular, it concerns the topological classification of structural defects in ordered materials. A discussion of the subject may be found in [7]. Fundamental principles of the topological classification scheme in the framework of broken symmetry have been given in [4].

While substantial progress for translationally invariant continuous media has been achieved (see [9, 5]), crystalline structures turned out to be more difficult. Two different approaches have been proposed, based on affine [8] and isometric [4] groups, respectively. As noted in [3], in the case of

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crystalline medium not every continuous map need correspond to a physical state. Physically admissible states should be restricted by appropriate compatibility conditions, which would express the relations between local states at infinitesimally close points of the medium. Such conditions might, in principle, render non–trivial homotopy classes physically not realizable, what would make homotopic classification ineffective.

In the present paper we propose appropriate compatibility conditions for 2D lattices. Although the problem makes sense also for higher dimensionalities, the 2D case is distinguished, and deserves separate consideration for several reasons. Firstly, the space R^2 admits natural complex structure, which converts it into C^1, endowed with powerful analytic properties. Secondly, as is well known from anyonic physics [11], the topological covering properties of planar systems are exceptional and more complicated (braid groups) than for other space dimensionalities. Moreover, 2D physical structures are of direct interest in surface physics, crystalline interfaces, high T_c superconducting CuO_2 planes, and in other physical situations where planar sub-structures play dominant role. The 2D case provides also a good point of departure for developing the 3D theory. For reasons of simplicity, we restrict our present considerations to Bravais lattices. Topological description of crystalline lattices of complex structure is given in [10].

2 The manifold of planar Bravais lattices

To discuss the topology of lattice distortions in a reasonably precise way, one needs a topological space whose points can be put into a bijective correspondence with the set of all ideal lattice states [8]. For 2D lattices it is a 6D topological manifold Λ

$$\Lambda \doteq G/\Gamma \tag{1}$$

where $G = \mathrm{GA}^+(2, R)$ and $\Gamma = \mathrm{SA}(2, Z)$. Taking into account the topology of G (Γ is then a discrete subgroup of G) one endows Λ with the quotient topology. In the above construction, two lattices are considered identical iff they coincide as subsets of the plane E^2.

We also make use of the standard representation of a lattice by an affine frame, consisting of a point $a \,\epsilon\, E^2$ and two base vectors a_K, $K = 1, 2$. It is, however, crucial to observe that the space of affine frames (which will be here identified with the affine group $\mathrm{GA}(2, R)$) is not equivalent to Λ. This

is due to the well known fact that, while an affine frame determines a unique lattice, the converse does not hold. Two different frames can determine the same lattice.

This defines an equivalence relation between the affine frames. Let

$$r^{(1)} = (a^{(1)}, a^{(1)}_{\ 1}, a^{(1)}_{\ 2}), \quad r^{(2)} = (a^{(2)}, a^{(2)}_{\ 1}, a^{(2)}_{\ 2}) \tag{2}$$

be a pair of such frames with the same (positive) orientation. Then $r^{(1)}$ and $r^{(2)}$ are equivalent iff there exists a unimodular matrix $A_K^{\ L}$ and a column b^L, both of integer components and such that

$$\begin{aligned} a^{(2)}_{\ K} &= A_K^{\ L} a^{(1)}_{\ L}, \\ b^{(2)} &= b^{(1)} + b^L a^{(1)}_{\ L}. \end{aligned} \tag{3}$$

In shorthand it can be put as

$$r^{(2)} = \gamma r^{(1)}, \quad \gamma \in \Gamma. \tag{4}$$

By a reference lattice we shall understand the lattice which under (1) corresponds to the unit matrix in G. The actual form of this lattice depends on the reference frame.

Let us briefly discuss the global structure of the manifold Λ. The notation $\mathrm{SA}(2, R)$ will be shortened here to H.

1. Λ can be represented as the topological product

$$\Lambda = R_+ \times \Sigma, \quad \Sigma = H/\Gamma. \tag{5}$$

The manifold Σ is composed of the lattices that are equi-areal with the reference lattice. Λ and Σ have identical homotopy type.

2. Λ (resp. Σ) is topologically covered by G (resp. H). In both cases the fibre of the covering coincides with Γ. In consequence Λ (or Σ) and G (or H) have identical homotopy properties for dimensions $n \geq 2$. The coverings carry the structure of differentiable manifold from the Lie groups G, H to the spaces Λ, Σ.

3. Λ is a homogeneous G–space, Σ is a homogeneous H–space. In both cases the stationary subgroup of the reference lattice equals Γ.

4. The action of the Euclidean isometries $E \subset G$ on Λ determines a fibration

$$p : \Lambda \to \Lambda/E \tag{6}$$

where Λ/E denotes the relevant space of orbits. The fibration p does not, however, satisfy the bundle property. Similiar construction holds for E, H and Σ.

The structure of the space of orbits Λ/E can be investigated by making use of the results given by Gruber [2]. The four strata of Λ/E correspond to the four 2D crystallographic systems.

3 Compatibility of the distortion fields

Let B be a 2D region occupied by a planar material structure and let

$$f : B \to \Lambda \tag{7}$$

be the distortion field in B. For our present purposes it is sufficient to consider connected open regions B of the form

$$B = \text{int } A \ \setminus \ \bigcup_{\iota \,\epsilon\, J} A_\iota \tag{8}$$

where ι runs through a finite index set J, while A and A_ι are contractible compact subsets of E^2, A_ι's being mutually disjoint subset of int A. The covering $G \to \Lambda$ guarantees then the existence of an open covering $\{B_\alpha\}$ of B and a collection of local fields

$$g_\alpha : B_\alpha \to G \tag{9}$$

which satisfy the equivalence relation

$$g_\beta(x) \,\epsilon\, \Gamma g_\alpha(x) \quad \text{for} \ \ x \,\epsilon\, B_\alpha \cap B_\beta \tag{10}$$

and correspond to the field (7). In this way the problem of geometric compatibility of a distortion field (7) reduces locally to the problem of geometric compatibility of appropriate fields of affine frames, which can be solved by differential-geometric methods.

To that effect we shall apply locally the approach presented in [6]. A differentiable field of affine frames defines a soldering form θ and a field of linear coframes ω which together determine an affine connection which,

projected into linear connections, is a teleparallelism. The corresponding affine curvature is composed of the translation part

$$D\theta = d\theta + \omega \wedge \theta \tag{11}$$

and the linear part

$$D\omega = d\omega + \frac{1}{2}[\,\omega, \omega\,] = 0 \tag{12}$$

(temporarily we suppress the index α). D stands here for the covariant exterior differentiation defined by our connection.

While the linear curvature $D\omega$ vanishes identically, the translation part $D\theta$ in general does not vanish. In geometric terms it defines the torsion $\tau = D\omega$ which, in turn, may be interpreted physically as the density of a certain continuous distribution of dislocations. In our case we take $\tau_\alpha = 0$ as the necessary and sufficient condition of local geometric compatibility in each B_α, which is equivalent to local holonomicity of the affine frame fields. It is essential to observe that the above condition is independent of the choice of a representative in the equivalence class (10). In consequence, the local geometric (in)compatibility characterizes the field (7).

For a simply-connected B the geometric compatibility implies that the distortion field f can be derived locally from a displacement field u. If $u \to 0$ smoothly, then $f \to \text{const}$ along a path of geometrically compatible distortion states.

Consider now a multiply-connected B. In spite of vanishing τ, the affine connection may have non-trivial holonomy for non-contractible loops, expressed by elements $h \,\epsilon\, \Gamma$. For a given distortion field f a loop from B is mapped into a loop in Λ which, in turn, can be (uniquely) lifted to a path in G which starts from the unit element $e \,\epsilon\, G$ and terminates in a certain (Burgers) element $g \,\epsilon\, G$. It is straightforward to verify that for geometrically compatible distortion fields f, the Burgers element g coincides with the holonomy element h.

Apart from the teleparallelism connection, one can also consider the Riemann–Cartan connection associated with a given frame field. By straightforward calculation one can verify that the geometric compatibility condition can be formulated in an alternative, although equivalent, way: the associated teleparallelism coincides with the associated Riemann–Cartan connection.

Note that the above stated criteria for geometric compatibility are directly valid also for higher dimensionalities and more general manifolds. In the next

section we shall show the existence of distortion fields in E^2 which are, at the same time, geometrically compatible and topologically non–trivial.

4 Existence of compatible representatives

Let us note that eqn. (8) implies the existence of a finite open covering of B by contractible sets B_α. For such a covering, if the distortion field f is compatible then each g_α is derivable from an immersion $w_\alpha : B_\alpha \to R^2$. Note, however, that this immersion need not be an embedding.

Now we can ask the question: do geometrically compatible and toplogically non–trivial distortions exist? To show that the answer is in the affirmative, consider the following multi–valued analytic function

$$w(z) = \frac{1}{2\pi i} \sum_{\iota \,\epsilon\, J} [(a_\iota (z - z_\iota) + c_\iota) \log(z - z_\iota) - (b_\iota (z - z_\iota)^* + d_\iota) \log(z - z_\iota)^*] \tag{13}$$

where $z_\iota \;\epsilon\; A_\iota$. For an appropriate covering $\{B_\alpha\}$ this function translates itself into a collection of immersions $w_\alpha : B_\alpha \to R^2$. This collection defines a geometrically compatible distortion field provided that a_ι, b_ι, and $c_\iota + d_\iota$ are complex integers such that

$$\mid a_\iota \mid^2 - \mid b_\iota \mid^2 = \; 1. \tag{14}$$

In consequence, the holonomy element h_ι associated with each $\iota \;\epsilon\; J$ equals the affine transformation defined by

$$\mathrm{Re} \begin{pmatrix} (a_\iota + b_\iota) & i(a_\iota - b_\iota) \\ -i(a_\iota + b_\iota) & (a_\iota - b_\iota) \end{pmatrix} \begin{pmatrix} x - x_\iota \\ y - y_\iota \end{pmatrix} + \begin{pmatrix} \mathrm{Re}(c_\iota + d_\iota) \\ \mathrm{Im}(c_\iota + d_\iota) \end{pmatrix}, \tag{15}$$

so that any $\gamma_\iota \;\epsilon\; \Gamma$ can be obtained in this way. The group identity is realized only by

$$a_\iota \;=\; 1, \;\; b_\iota \;=\; c_\iota + d_\iota \;=\; 0 \tag{16}$$

so that all the remaining elements correspond to non–trivial homotopy classes. Moreover, the immersions $w_\alpha : B_\alpha \to R^2$ can be made embeddings by a finite refinement of the covering $\{B_\alpha\}$.

The above formulation allows us to draw also a contrasting conclusion concerning the isometric approach to crystalline defects. When in (1) the

group G is restricted to the Euclidean isometries of the plane, and Γ is restricted to the crystallographic space group of the reference lattice, then the frames (2) can be chosen orthogonal. In that case the associated metrics can be represented by the unit matrix, what makes the Christoffel symbols vanish for compatible configurations. In consequence the teleparallelism connection coefficients also vanish, and only homogeneous states survive. As a result, in the isometric approach the geometrically compatible distortions are always topologically trivial. This is in contrast with the situation in the affine theory, which admits a rich variety of topological, non-trivial distortion fields.

The above results can further be strenghtened by taking

$$w(z) \,=\, w_1(z,z^*) + w_2(z,z^*) \tag{17}$$

where $w_1(z,z^*)$ is given by eqn. (13), and the function $w_2(z,z^*)$ is, for every $z \in B$, holomorhic with respect to z and anti–holomorphic with respect to z^*. By appropriate choice of meromorphic terms in $w_2(z,z^*)$ one obtains geometrically compatible distortion fields characterized by non–zero winding numbers.

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